

Ecotox Report for Case # P-18-0136

General

CBI: [REDACTED]	Report Status: Complete
Status 11/19/2018	CRSS Date:
Date:	
SAT	SAT
Date:	Chair:
Consolidated N	Consolidated Set:
PMN:	
Ecotox [REDACTED]	
Related Cases: [REDACTED]	
Health	
Related Cases:	
Submitter: [REDACTED]	
CAS Number:	
Chemical	
Name: [REDACTED]	
Use: [REDACTED]	
[REDACTED]. The anion portion of the	
PMN material is [REDACTED]. All analogs are dyes for [REDACTED]	
Trade Name: MKP	
1003	
PV-max(kg/yr): [REDACTED]	Ecotox Assessor: Kim, Anne

Fate Summary Statement

Fate P-18-0136
Summary FATE:
Statement:
Solid
Log Kow = 1.74 (M)
S = 2.067 g/L at 25 °C (M)
VP <
1.0E-6 torr at 25 °C (E)
BP > 400 °C (E)
H < 1.00E-8
(E)
POTW removal (%) = 0-25 via sorpton; Analog [REDACTED]
[REDACTED]:
OECD 301B(Mod Sturm CO2 ev): 2-3%/28d
NRB.

Time for complete ultimate aerobic biodeg > mo
Sorption to
soils/sediments = low - moderate
PBT Potential: P3B1
*CEB FATE:
Migration to ground water = moderate - rapid
Bioconcentration factor to
be put into E-FAST: 3

Physical Chemical Information

Molecular Weight:	
Wt% < 500:	Wt% < 1000:
Physical State - Neat:	
Melting Point:	Melting Point (est):
MP (EPI):	
Vapor Pressure:	Vapor Pressure (est): <0.000001
VP (EPI):	
Water Solubility: 2.067	Water Solubility (est):
Water Solubility (EPI):	
Henry's Law::	
Log Koc:	Log Koc (EPI):
Log Kow:	Log Kow (EPI):
Log Kow Comment:	

SAT Concern Level

Ecotox Rating (1):	2
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	

Ecotox Route of Exposure: All releases to water

Ecotox Comments

Exposure Based Review (Eco):
Ecotox Comments:
Exposure Based Testing:

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall):	Rating Values	Rating Description				Comment
Condition	1	2	3	4		
Fish BCF:						
Log Fish BCF:						
WWT/POTW Sorption:	Low	Moderate	Strong	V. Strong		
WWT/POTW Stripping:	Extensive	Moderate	Low	Negligible		
Biodegradation Removal:	Unknown	High	Moderate	Negligible		
Biodegradation Destruction:	Unknown	Complete	Partial	—		
Aerobic Biodeg Ult:	<= Days	Weeks	Months	> Months		
Aerobic Biodeg Prim:	<= Days	Weeks	Months	> Months		
Anaerobic Biodeg Ult:	<= Days	Weeks	Months	> Months		
Anaerobic Biodeg Prim:	<= Days	Weeks	Months	> Months		

Removal in WWT/POTW (Overall): Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:		V. Strong	Strong	Moderate	Low	
Migration to Ground Water:		Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
Bio Comments:						
Fate Comments:						

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	>43		P: Analogue: same as [REDACTED]
Daphnid	48-h	LC50	2.8	1.93	P: Analogue: [REDACTED] M: PMN
Green Algae	96-h	EC50	1.2		P: Analogue: [REDACTED]
Fish	-	Chronic Value	>4.3		P: [REDACTED]
Daphnid	-	Chronic Value	0.28	0.193	P: [REDACTED]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Green Algae	-	Chronic Value	<0.21		<div> <div></div> <div>M: <div></div></div> <div>P: Analog: <div></div></div> <div></div> </div>
<p>Ecotox Value Predictions are based on data for the PMN substance and analogue <div></div> MW <div></div>; Log Kow = 1.74 (M); solid with an unknown</p> <p>MP (P); S = 2067 mg/L (M); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO₃; and TOC <2.0 mg/L.</p> <p>Ecotoxicity Test Data Results</p> <p>Case</p> <p>Number: P-18-0136</p> <p>Chemical Name: <div></div></p> <p><div></div></p> <p>CAS RN: <div></div></p> <p>Trade Name: MKP 1003</p> <p>Initial Data</p> <p>Review</p> <p>Invertebrate Ecotoxicity Test:</p> <p>Eurofins Agrosience</p> <p>Services EcoChem/Ecotox GmbH conducted a 48-hour acute toxicity test in the water flea (<i>Daphnia magna</i>) with P-18-0136 (purity not stated; mono/disulfonic acid ratio: 16.1:83.9) under semi-static conditions with 24-hour renewal. The water solubility of the test item was reported to be 206.7 mg/L. This study followed OECD test guideline No. 202 (2004). Following a range-finding test, four replicates of five <i>D. magna</i> were exposed to a dilution water control (Elendt M4 medium) or the test substance at nominal concentrations of 0, 0.427, 0.939, 2.07, 4.55, and 10 mg/L. Corresponding mean measured test concentrations (calculated as the geometric mean of the sum of the <div></div> components) were 0.307, 0.657, 1.47, 3.46, and 6.80 mg/L (68-76% of nominal), as determined by HPLC-MS/MS analysis, (LOQ = 0.07 mg/L). To prepare the test solutions, a stock solution (10 mg/L) was prepared by adding an appropriate amount of test item to a volumetric flask, adding dilution water, and stirring/homogenizing for 120 minutes. The solution was allowed to settle for 5 minutes following the stirring period. Following this period, the solution was rose-colored and fine particles of</p>					

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
				<p>substance were visible. Test solutions at the remaining nominal test concentrations were prepared by dilution of the appropriate test solutions. At concentrations of ≥ 0.939 mg/L, daphnids were observed to be collocated. Flakes of test substance were observed at the bottom of the test vessel in the 4.55 and 10 mg/L test solutions at 24 and 48 hours. Over the course of the study, temperature ranged from 19.7-21.0°C, pH ranged from 7.76-8.15, and dissolved oxygen ranged from 8.7-9.1 mg/L. Dilution water hardness was 214 mg/L as CaCO₃. A loading rate of 100 daphnids/L was calculated. Percent immobility at concentrations of 0 (control), 0.427, 0.939, 2.07, 4.55, and 10 mg/L was 0%, 5%, 30%, 35%, 70%, and 95%, respectively. Based on mean measured concentrations, the 48-hour EC₅₀ was 1.93 mg/L.</p> <p>48-hour EC₅₀ = 1.93 mg/L</p> <p>The test substance information and study summaries below are for an analogous chemical, not the actual PMN substance. Although not specified by the submitter, the tested substance is the same as PMN substance</p> <p>Chemical Name:</p> <p>Trade Name:</p> <p>Fish Ecotoxicity Test:</p> <p>Institute of Pesticide and Environmental Toxicology, Zhejiang University (China) conducted a 96-hour acute toxicity test in zebrafish (<i>Brachydanio rerio</i>) with the analog test substance (purity: >99%) under static conditions. This study followed OECD test guideline No. 203 (1992). The test substance was not completely soluble in test medium at the concentrations tested. Single replicates of ten <i>B. rerio</i> were exposed to a dilution water control (dechlorinated tap water) or a filtered test solution prepared at a loading rate of 100 mg/L. The corresponding mean measured test concentration was 42.88 mg/L, as determined by HPLC analysis with UV/VIS detection, (LOD = 0.1 mg/L). To prepare the test solution, 1000 mg of test item was added to 10 L of dilution water. After stirring for 8 hours, the mixture was filtrated with qualitative filter paper to</p>

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
		<p>remove undissolved test substance particles. Over the course of the study, temperature ranged from 23.2-24.6°C, pH ranged from 5.76-6.42, and dissolved oxygen ranged from 6.44-7.25 mg/L. Dilution water hardness was 60-80 mg/L as CaCO₃. A biomass loading rate of 0.18 g fish/L was calculated. No mortalities or observable symptoms occurred in the control or test group. Based on mean measured concentrations, the 96-hour LC₅₀ was > 42.88 mg/L.</p> <p>96-hour LC₅₀ > 42.88 mg/L</p> <p>Algal Ecotoxicity Test: NOTOX B.V. conducted a 72-hour acute toxicity test in green algae (<i>Pseudokirchneriella subcapitata</i>) with the analog test substance (purity: >95%) under static conditions. The water solubility of the two anions was determined to be 412 mg/L and 73 mg/L, respectively. The test substance was not completely soluble in test medium at a loading rate of 100 mg/L. This study followed OECD test guideline No. 201 (2006), EEC directive 92/69, Part C (1992), ISO International Standard 8692 (2004), and OECD test guideline No. 23 (2000). Following a range-finding test, three replicates of <i>P. subcapitata</i> (1x10⁴ cells/mL) were exposed to test substance concentrations of 0.32, 1, 3.2, 10, 32, or 100% of a water soluble fraction (WSF) prepared at a nominal loading rate of 100 mg test item/L. Additionally, six control replicates of <i>P. subcapitata</i> were exposed to dilution water only (M2 medium). Test substance measurements were performed for the cation and two anionic parts (peaks 1 and 2) of the test substance via HPLC analysis (LOD = 0.19-0.28 mg/L). Mean measured test substance concentrations ranged from 99-124% of nominal based on the cation, 101-124% of nominal based on anionic peak 1, and 25-93% of nominal based on anionic peak 2. Test substance concentrations based on the anionic peak 2 were significantly lower at the start of the test and, especially at the lower concentrations, did not remain stable. Taking the worst case scenario into account, effect parameters were based on the average exposure concentrations of test substance based on anionic part peak 2 (<LOQ, <LOQ, 0.21, 0.86, 5.4, and 23 mg/L in the 0.32, 1, 3.2, 10, 32, and 100% WSFs, respectively). The algal cultures were illuminated with a light intensity of 110-115 µE/m²/s, with constant shaking. A loading rate of 100 mg/L was first prepared by applying a 15-minute treatment of ultrasonic waves, followed by 30-35 minutes of magnetic stirring to obtain maximum solubility in the test medium. Subsequently, this mixture was left to stabilize for 2.0-2.25 hours, after which the water soluble fraction (WSF) was siphoned off. The WSF prepared for the final test was left to stabilize for another 30 minutes and a second WSF was siphoned off because very small particles were observed in the first one. The lower test concentrations were prepared by subsequent</p>		

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
				<p>dilutions of the WSF in test medium. The final test solutions were all clear and ranged from colorless to dark pink. Over the course of the study, temperature ranged from 21.9-23.1°C and pH ranged from 7.9-8.3. Dilution water hardness was 24 mg/L as CaCO₃. The mean cell density of control cultures increased by a factor of 328.5 within 72 hours. Based on mean measured concentrations (of the anionic peak 2), the 72-hour EC₅₀ for growth rate was 12 mg/L. The 72-hour NOEC and LOEC values for growth rate were 0.21 mg/L and 0.86 mg/L, respectively; the calculated ChV was 0.42 mg/L. The 72-hour EC₅₀ for yield was 1.2 mg/L. The 72-hour NOEC and LOEC values for yield were <0.21 mg/L and 0.21 mg/L, respectively.</p> <p>72-hour EC₅₀ (growth rate) = 12 mg/L 72-hour NOEC (growth rate) = 0.21 mg/L 72-hour LOEC (growth rate) = 0.86 mg/L</p> <p>72-hour ChV (growth rate) = 0.42 mg/L</p> <p>72-hour EC₅₀ (yield) = 1.2 mg/L 72-hour NOEC (yield) < 0.21 mg/L 72-hour LOEC (yield) = 0.21 mg/L</p> <p>██████████. (sponsor) submitted three toxicity studies on P-18-0136. The daphnia study was on the PMN, and fish and algal studies were on an analogous chemical ██████████ (the tested substance is the same as PMN substance. These studies were considered to be acceptable for the purposes of the acute and chronic concentration of concern (COC) determination.</p> <p>Based on submitted experimental data on P-18-0136 and its analogue, the acute COC for P-18-0136 is 300 ppb (1200 ppb / 4 (uncertainty factor)) for algae. The chronic COC for P-18-0136 is 19 ppb (193 ppb / 10 (uncertainty factor)), based on the submitted test data for daphnia.</p> <p>Acute COC = 300 ppb Chronic COC = 19 ppb</p>

Test organism	Test Type	Test Endpoint	Predicted	Experimental Comments
Ecotox Reviewer: A. Kim Date: 4/25/2018				

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	1200	4	300	Algal EC50
Chronic Aquatic(ppb):	193	10	19	Daphnid ChV
Factors	Values	Comments		
SARs:				
SAR Class:				
TSCA NCC Category?	Acid Dyes and Amphoteric Dyes			

Recommended Potentially Useful

Testing: Information: None

Ecotox Environmental

Factors Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data for the new chemical substance and hazard data on analogous chemical () Substance falls within the TSCA New Chemicals Category of Acid Dyes and Amphoteric Dyes. Acute toxicity values estimated for fish, aquatic invertebrates, and algae are >43 mg/L (analogue data), 1.93 mg/L (PMN data), and 1.2 mg/L (analogue data), respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are >4.3 mg/L (using ACR 10 of analogue), 0.193 mg/L (using ACR 10 of PMN), and <0.21 mg/L (analog data), respectively. These toxicity values indicate that the new chemical substance is expected to have moderate environmental hazard. Application of assessment factors of 4 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 0.300 mg/L (300 ppb) and 0.019 mg/L (19 ppb), respectively.

Environmental Risk: Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks to the environmental were not identified due to no releases to water.

Comments/Telephone Log

Artifact	Update/Upload Time
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